Notes for AA214, Chapter 6

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Linear Multistep Methods

The Linear Multistep Methods (LMM's) are probably the most natural extension to time marching of the space differencing schemes.

$$\sum_{k=1-K}^{1} \alpha_k u_{n+k} = h \sum_{k=1-K}^{1} \beta_k u'_{n+k}$$

Applying the representative ODE, $u' = \lambda u + a e^{\mu t}$, the charactistic polynominals $P(E)$ and $Q(E)$

$$\begin{aligned}\left[\left(\sum_{k=1-K}^{1} \alpha_k E^k\right) - \left(\sum_{k=1-K}^{1} \beta_k E^k\right) h\lambda\right] u_n &= h\left(\sum_{k=1-K}^{1} \beta_k E^k\right) a e^{\mu h n} \\ [P(E)]\, u_n &= Q(E) a e^{\mu h n}\end{aligned}$$

Consistency requires that $\sigma \to 1$ as $h \to 0$ which is met if

$$\sum_k \alpha_k = 0 \quad \text{and} \quad \sum_k \beta_k = \sum_k (K + k - 1)\alpha_k$$

"Normalization" results in $\sum_k \beta_k = 1$

Families of Linear Multistep Methods

1. Adams-Moulton family

$$\alpha_1 = 1, \qquad \alpha_0 = -1, \qquad \alpha_k = 0, \qquad k = -1, -2, \cdots$$

2. Adams-Bashforth family has the same α's with the additional constraint that $\beta_1 = 0$.

3. Three-step Adams-Moulton method can be written in the following form

$$u_{n+1} = u_n + h(\beta_1 u'_{n+1} + \beta_0 u'_n + \beta_{-1} u'_{n-1} + \beta_{-2} u'_{n-2})$$

   Taylor tables can be used to find classes of second, third and fourth order methods.

4. For example, with $\beta_1 = 0$ and

$$\beta_0 = 23/12, \qquad \beta_{-1} = -16/12, \qquad \beta_{-2} = 5/12$$

   produces the third-order Adams-Bashforth method.

Examples of Linear Multistep Methods

Explicit Methods

$$
\begin{aligned}
u_{n+1} &= u_n + hu'_n && \text{Euler} \\
u_{n+1} &= u_{n-1} + 2hu'_n && \text{Leapfrog} \\
u_{n+1} &= u_n + \tfrac{1}{2}h\left[3u'_n - u'_{n-1}\right] && \text{AB2} \\
u_{n+1} &= u_n + \tfrac{h}{12}\left[23u'_n - 16u'_{n-1} + 5u'_{n-2}\right] && \text{AB3}
\end{aligned}
$$

Implicit Methods

$$
\begin{aligned}
u_{n+1} &= u_n + hu'_{n+1} && \text{Implicit Euler} \\
u_{n+1} &= u_n + \tfrac{1}{2}h\left[u'_n + u'_{n+1}\right] && \text{Trapezoidal (AM2)} \\
u_{n+1} &= \tfrac{1}{3}\left[4u_n - u_{n-1} + 2hu'_{n+1}\right] && \text{2nd-order Backward} \\
u_{n+1} &= u_n + \tfrac{h}{12}\left[5u'_{n+1} + 8u'_n - u'_{n-1}\right] && \text{AM3}
\end{aligned}
$$

Two-Step Linear Multistep Methods

1. Minimal storage requirements for high-resolution CFD problems restrict methods to two time levels.

2. Most general scheme $(1+\xi)u_{n+1} = [(1+2\xi)u_n - \xi u_{n-1}] + h\,[\,\theta u'_{n+1} + (1-\theta+\varphi)u'_n - \varphi u'_{n-1}]$

3. Examples:

θ	ξ	φ	Method	Order
0	0	0	Euler	1
1	0	0	Implicit Euler	1
1/2	0	0	Trapezoidal or AM2	2
1	1/2	0	2nd Order Backward	2
3/4	0	−1/4	Adams type	2
1/3	−1/2	−1/3	Lees	2
1/2	−1/2	−1/2	Two–step trapezoidal	2
5/9	−1/6	−2/9	A–contractive	2
0	−1/2	0	Leapfrog	2
0	0	1/2	AB2	2
0	−5/6	−1/3	Most accurate explicit	3
1/3	−1/6	0	Third–order implicit	3
5/12	0	1/12	AM3	3
1/6	−1/2	−1/6	Milne	4

4. Both er_μ and er_λ are reduced to $0(h^3)$ if $\varphi = \xi - \theta + \frac{1}{2}$

5. The class of all 3rd-order methods $\xi = 2\theta - \frac{5}{6}$

6. Unique fourth-order method is found by setting $\theta = -\varphi = -\xi/3 = \frac{1}{6}$.

Predictor-Corrector Methods

1. Predictor-corrector methods are composed of sequences of linear multistep methods.

2. Simple one-predictor, one-corrector scheme

$$\begin{aligned}\tilde{u}_{n+\alpha} &= u_n + \alpha h u'_n \\ u_{n+1} &= u_n + h\big[\beta \tilde{u}'_{n+\alpha} + \gamma u'_n\big]\end{aligned}$$

3. α, β and γ are arbitrary parameters.

$$\begin{aligned}P(E) &= E^\alpha \cdot \left[E - 1 - (\gamma+\beta)\lambda h - \alpha\beta\lambda^2 h^2\right] \\ Q(E) &= E^\alpha \cdot h \cdot [\beta E^\alpha + \gamma + \alpha\beta\lambda h]\end{aligned}$$

4. Second-order accuracy: *both* er_λ and er_μ must be $O(h^3)$.

5. Leads to: $\gamma + \beta = 1 \quad ; \quad \alpha\beta = \frac{1}{2}$

6. Second-order accurate predictor-corrector sequence for any α

$$\begin{aligned}\tilde{u}_{n+\alpha} &= u_n + \alpha h u'_n \\ u_{n+1} &= u_n + \frac{1}{2} h \left[\left(\frac{1}{\alpha}\right)\tilde{u}'_{n+\alpha} + \left(\frac{2\alpha - 1}{\alpha}\right) u'_n\right]\end{aligned}$$

Predictor-Corrector Methods: Examples

1. The Adams-Bashforth-Moulton sequence for $k = 3$

$$\begin{aligned}\tilde{u}_{n+1} &= u_n + \frac{1}{2}h\big[3u'_n - u'_{n-1}\big]\\ u_{n+1} &= u_n + \frac{h}{12}\big[5\tilde{u}'_{n+1} + 8u'_n - u'_{n-1}\big]\end{aligned}$$

2. The Gazdag method

$$\begin{aligned}\tilde{u}_{n+1} &= u_n + \frac{1}{2}h\big[3\tilde{u}'_n - \tilde{u}'_{n-1}\big]\\ u_{n+1} &= u_n + \frac{1}{2}h\big[\tilde{u}'_n + \tilde{u}'_{n+1}\big]\end{aligned}$$

3. The Burstein method $\alpha = 1/2$ is

$$\begin{aligned}\tilde{u}_{n+1/2} &= u_n + \frac{1}{2}hu'_n\\ u_{n+1} &= u_n + h\tilde{u}'_{n+1/2}\end{aligned}$$

4. MacCormack's method

$$\begin{aligned}\tilde{u}_{n+1} &= u_n + hu'_n\\ u_{n+1} &= \frac{1}{2}[u_n + \tilde{u}_{n+1} + h\tilde{u}'_{n+1}]\end{aligned}$$

Runge-Kutta Methods

1. Runge-Kutta method of order k (up to 4th order), the principal (and only) σ-root is given by

$$\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \cdots + \frac{1}{k!}\lambda^k h^k$$

2. To ensure kth order accuracy, the method must have $er_\mu = O(h^{k+1})$

3. General RK(N) scheme

$$\begin{aligned}
\widehat{u}_{n+\alpha} &= u_n + \beta h u'_n \\
\tilde{u}_{n+\alpha_1} &= u_n + \beta_1 h u'_n + \gamma_1 h \widehat{u}'_{n+\alpha} \\
\overline{u}_{n+\alpha_2} &= u_n + \beta_2 h u'_n + \gamma_2 h \widehat{u}'_{n+\alpha} + \delta_2 h \tilde{u}'_{n+\alpha_1} \\
u_{n+1} &= u_n + \mu_1 h u'_n + \mu_2 h \widehat{u}'_{n+\alpha} + \mu_3 h \tilde{u}'_{n+\alpha_1} + \mu_4 h \overline{u}'_{n+\alpha_2}
\end{aligned}$$

4. Total of 13 free parameters, where the choices for the time samplings, α, α_1, and α_2, are not arbitrary.

$$\begin{aligned}
\alpha &= \beta \\
\alpha_1 &= \beta_1 + \gamma_1 \\
\alpha_2 &= \beta_2 + \gamma_2 + \delta_2
\end{aligned}$$

Runge-Kutta Methods

1. Ten (10) free parameters remain to obtain various levels of accuracy.
2. Finding $P(E)$ and $Q(E)$ and then eliminating the β's results in the four conditions

$$\begin{aligned}
\mu_1 + \mu_2 + \mu_3 + \mu_4 &= 1 && (1)\\
\mu_2\alpha + \mu_3\alpha_1 + \mu_4\alpha_2 &= 1/2 && (2)\\
\mu_3\alpha\gamma_1 + \mu_4(\alpha\gamma_2 + \alpha_1\delta_2) &= 1/6 && (3)\\
\mu_4\alpha\gamma_1\delta_2 &= 1/24 && (4)
\end{aligned}$$

3. Guarantee that the five terms in σ exactly match the first 5 terms in the expansion of $e^{\lambda h}$.
4. To satisfy the condition that $er_\mu = O(h^5)$

$$\begin{aligned}
\mu_2\alpha^2 + \mu_3\alpha_1^2 + \mu_4\alpha_2^2 &= 1/3 && (3)\\
\mu_2\alpha^3 + \mu_3\alpha_1^3 + \mu_4\alpha_2^3 &= 1/4 && (4)\\
\mu_3\alpha^2\gamma_1 + \mu_4(\alpha^2\gamma_2 + \alpha_1^2\delta_2) &= 1/12 && (4)\\
\mu_3\alpha\alpha_1\gamma_1 + \mu_4\alpha_2(\alpha\gamma_2 + \alpha_1\delta_2) &= 1/8 && (4)
\end{aligned}$$

5. Gives 8 equations for 10 unknowns.

RK4 Method

1. Storage requirements and work estimates allow for a variety of choices for the remaining 2 parameters.

2. "Standard" 4^{th} order Runge-Kutta method expressed in predictor-corrector form

$$
\begin{aligned}
\widehat{u}_{n+1/2} &= u_n + \frac{1}{2} h u'_n \\
\tilde{u}_{n+1/2} &= u_n + \frac{1}{2} h \widehat{u}'_{n+1/2} \\
\overline{u}_{n+1} &= u_n + h \tilde{u}'_{n+1/2} \\
u_{n+1} &= u_n + \frac{1}{6} h \left[u'_n + 2\left(\widehat{u}'_{n+1/2} + \tilde{u}'_{n+1/2} \right) + \overline{u}'_{n+1} \right]
\end{aligned}
$$

3. Notice that this represents the simple sequence of conventional linear multistep methods

$$
\left.
\begin{array}{l}
\text{Euler Predictor} \\
\text{Euler Corrector} \\
\text{Leapfrog Predictor} \\
\text{Milne Corrector}
\end{array}
\right\} \equiv RK4
$$